Flow Chart

Any Protein
Coordinates
(x,y,z)

100

Mel Script

102

Generate Three-
Dimensional
Image of that Protein

104

FIG. 1

```
IDENTIFY 3D STRUCTURE
OF PROTEING                     ── 202


GENERATE POSITION DATA: (X, Y, Z)
COORDINATES FOR STRUCTURE       ── 204


CONVERT X, Y, Z
COORDINATES TO
MEL SCRIPT                      ── 206


GENERATE MODEL OF
ANIMATION OF PROTEIN            ── 208


DISPLAY                         ── 210
```
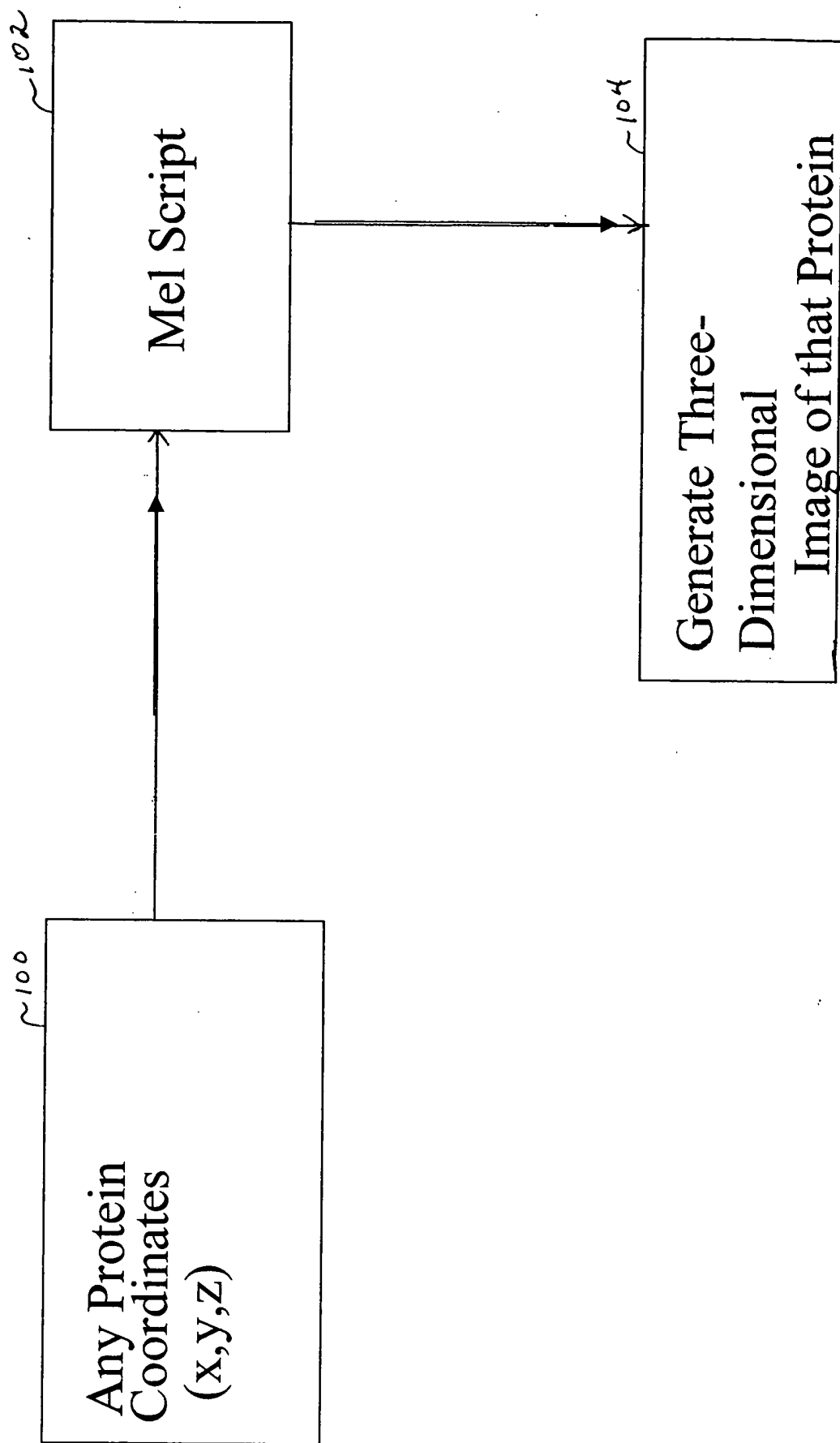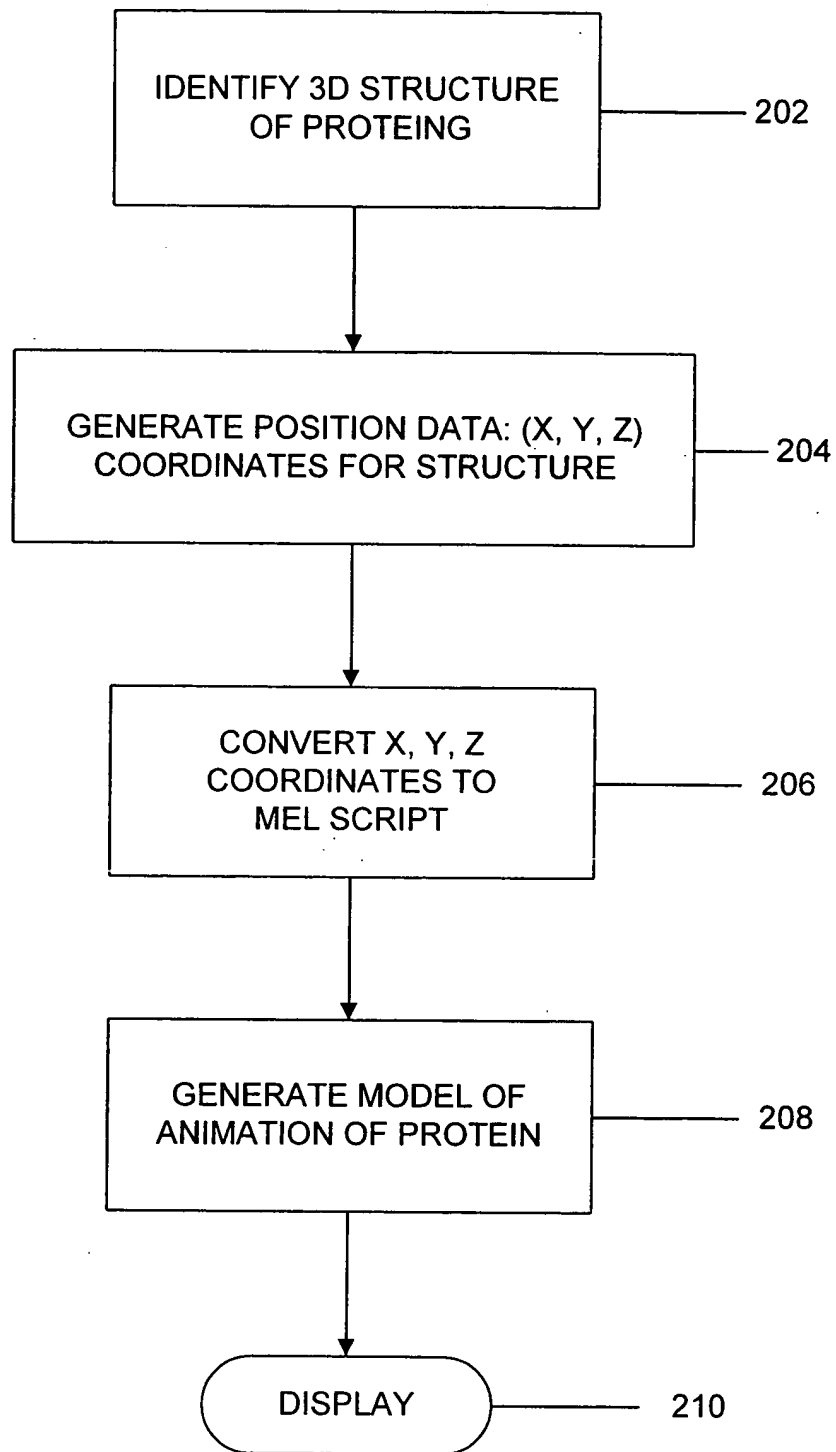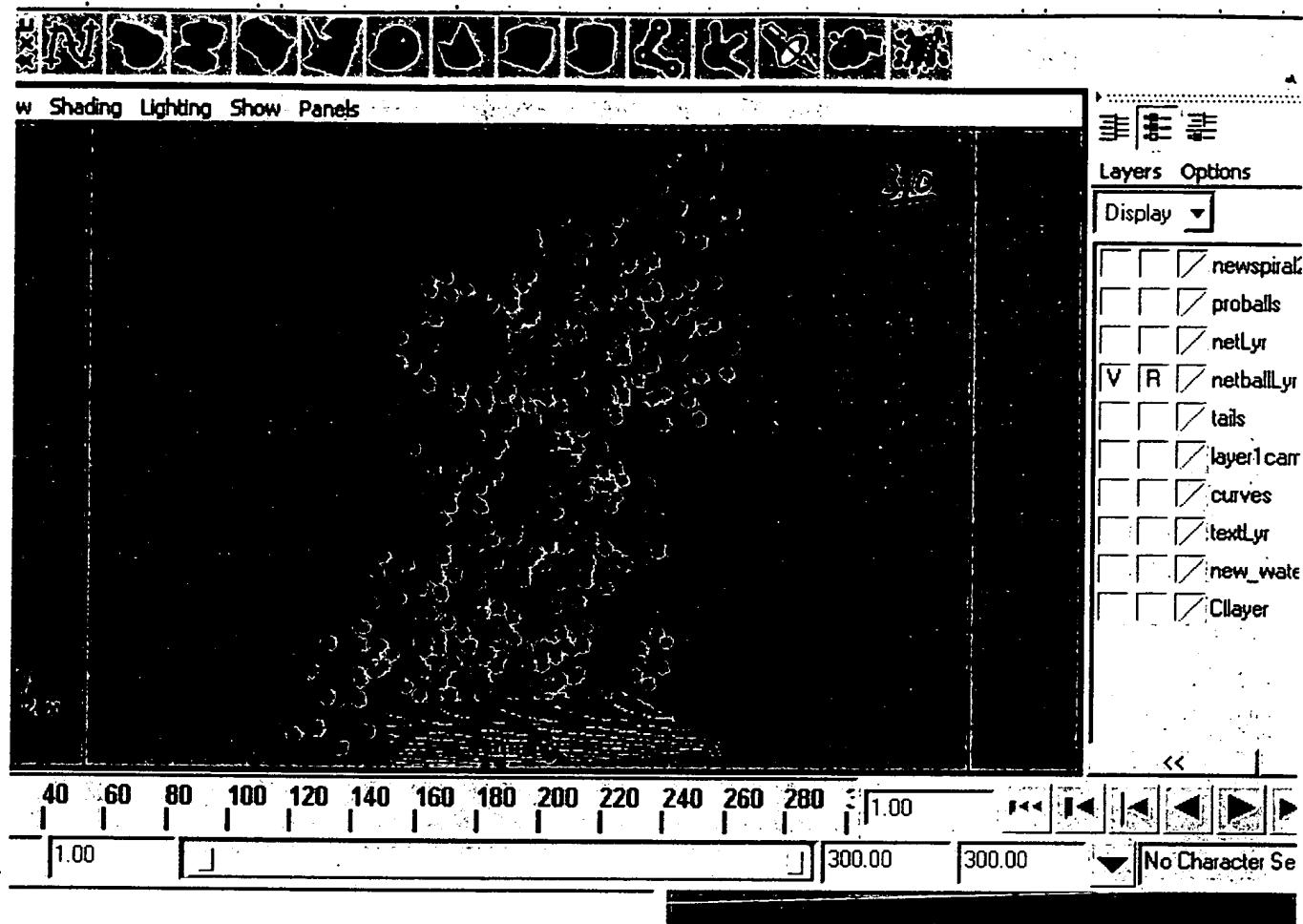
200

Fig. 2

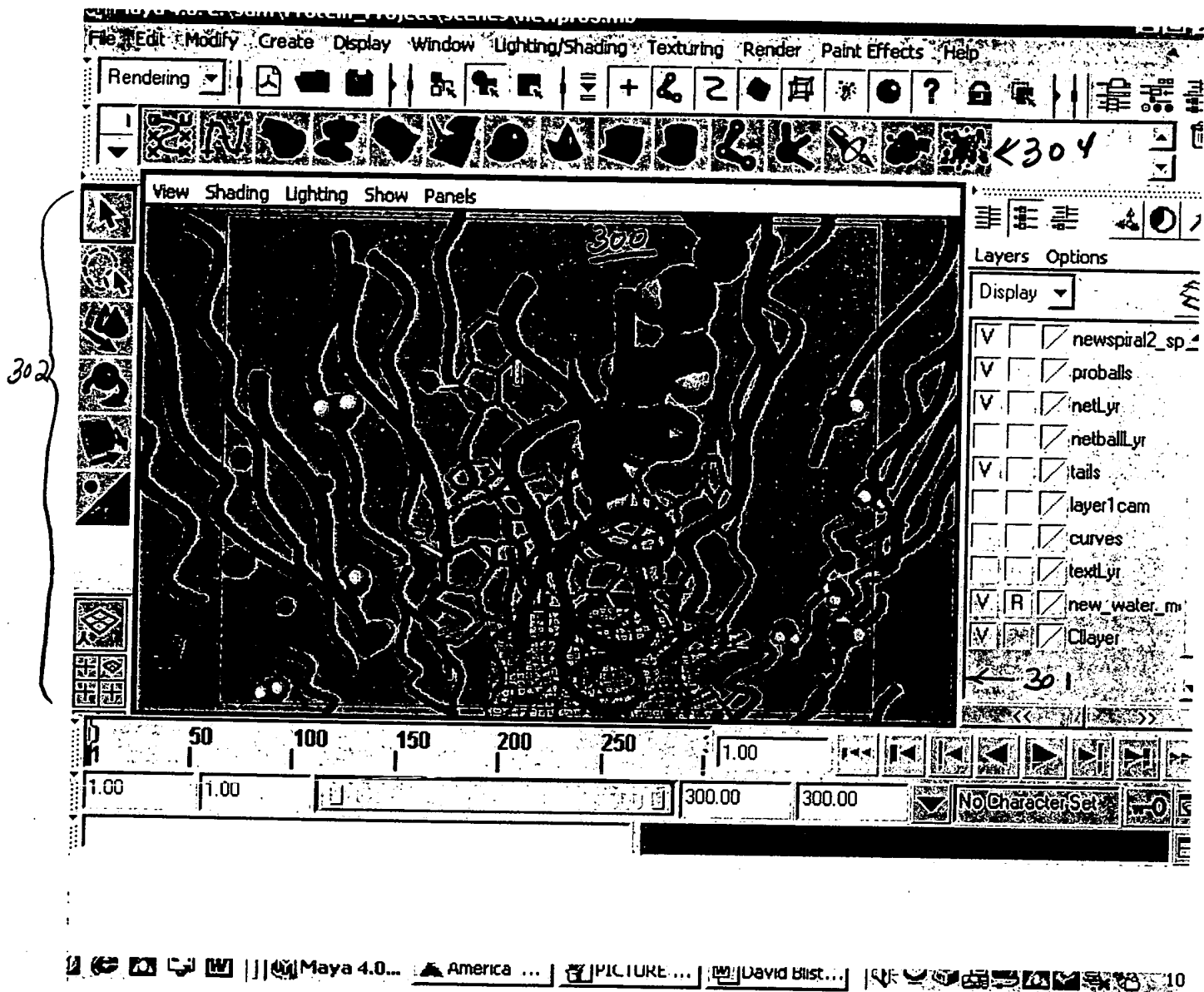Spheres generated from the mel script before they were connected

FIG. 3B

FIG. 3A

```
          ┌────────────────────────────────┐
          │  GENERATE INDIVIDUAL SPHERES    │──── 402
          │  FOR A FIRST LAYER             │
          └────────────────────────────────┘
                        │
                        ▼
               ┌──────────────────┐
               │  CONNECT THE     │──── 404
               │  SPHERES         │
               └──────────────────┘
                        │
                        ▼
              ┌───────────────────┐
              │ PRODUCE AN IMAGE  │──── 406
              │ FOR FIRST LAYER   │
              └───────────────────┘
                        │
                        ▼
              ┌───────────────────┐
              │ CHECK FOR         │──── 408
              │ ACCURACY          │
              └───────────────────┘
                        │
                        ▼
            ┌─────────────────────────┐
            │ PRODUCE THE NEXT LAYER  │──── 410
            │ BY GENERATIONS,         │
            │ SPHERES, ETC.           │
            └─────────────────────────┘
                        │
                        ▼
              ┌───────────────────┐
              │ ADD TO PRIOR      │──── 412
              │ LAYER             │
              └───────────────────┘
                        │
                        ▼
                  ◇ 414
              ┌─────────┐
              │   IS    │        NO
              │ PORTION │──────────────┐
              │COMPLETE?│              │
              └─────────┘              │
                   │                   │
              YES ──── 418             │
                   │                   │
                   ▼                   │
              ┌───────────────────┐    │
              │ EXAMINE ANIMATION │──── 420
              └───────────────────┘
                   │
              GO TO
              STEP 422
                   │
                   ▼
```
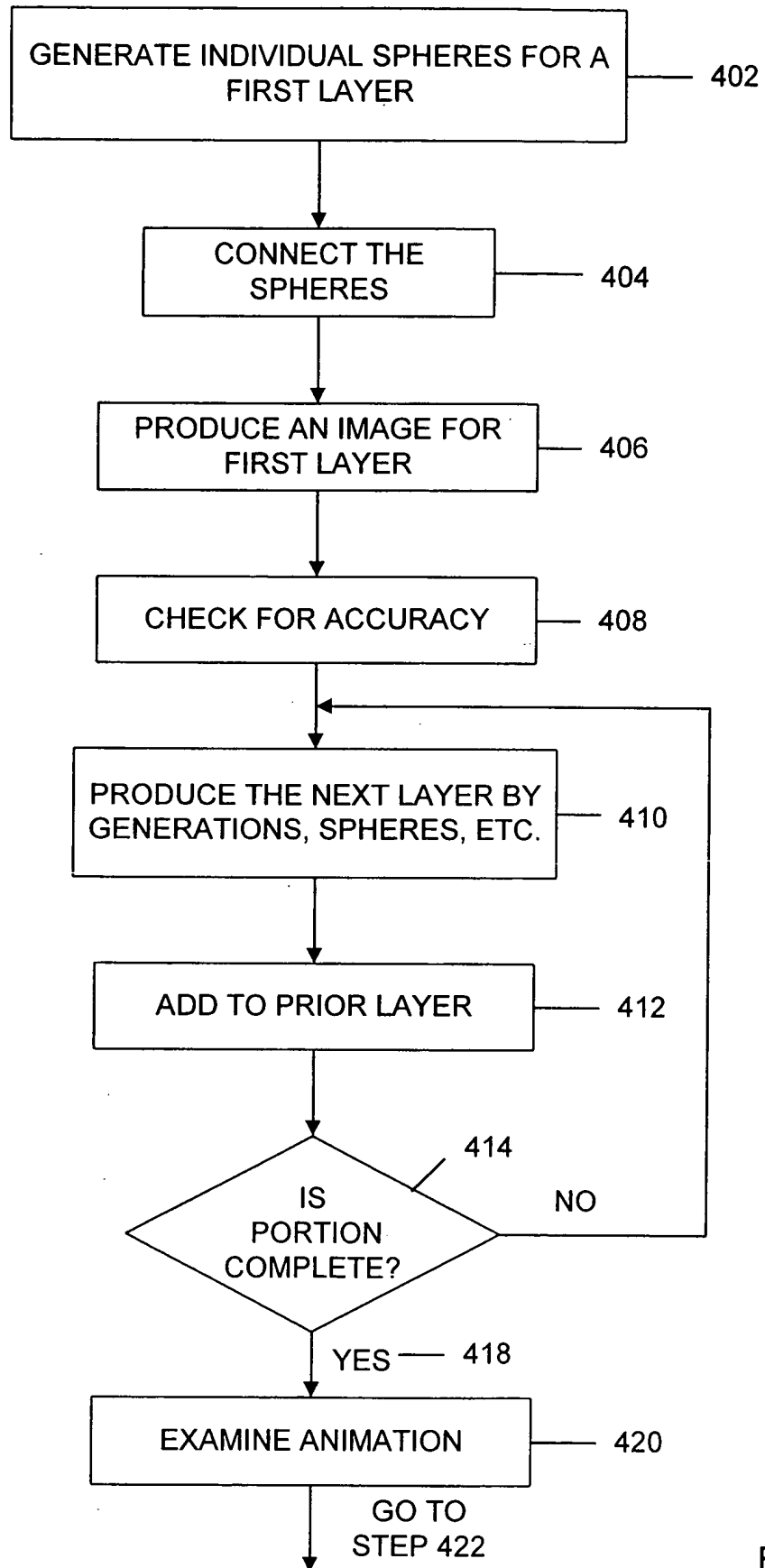
GENERATE INDIVIDUAL SPHERES FOR A FIRST LAYER — 402

CONNECT THE SPHERES — 404

PRODUCE AN IMAGE FOR FIRST LAYER — 406

CHECK FOR ACCURACY — 408

PRODUCE THE NEXT LAYER BY GENERATIONS, SPHERES, ETC. — 410

ADD TO PRIOR LAYER — 412

IS PORTION COMPLETE? — 414   NO

YES — 418

EXAMINE ANIMATION — 420

GO TO STEP 422

Fig. 4A

400

FROM
420

PROVIDE KEY FRAME — 424

ADD LIGHTING — 426

CHOOSE CAMERA, FILE, ETC. — 428

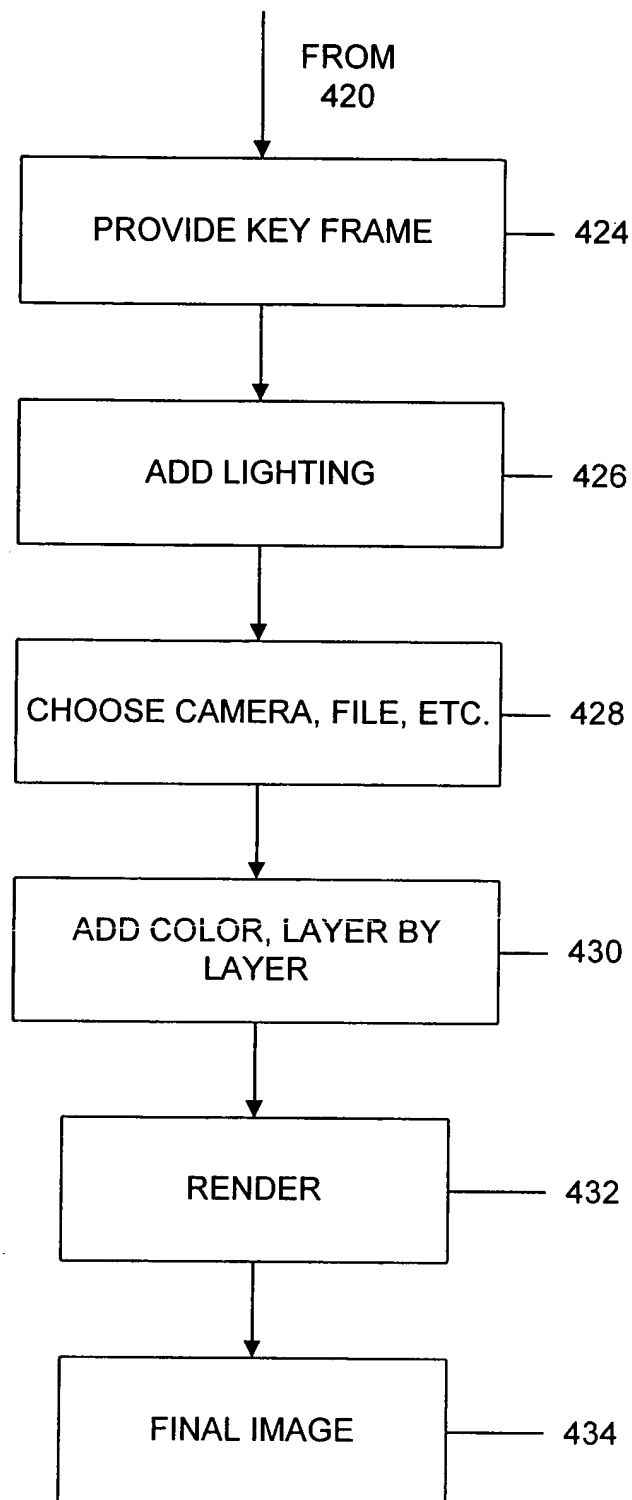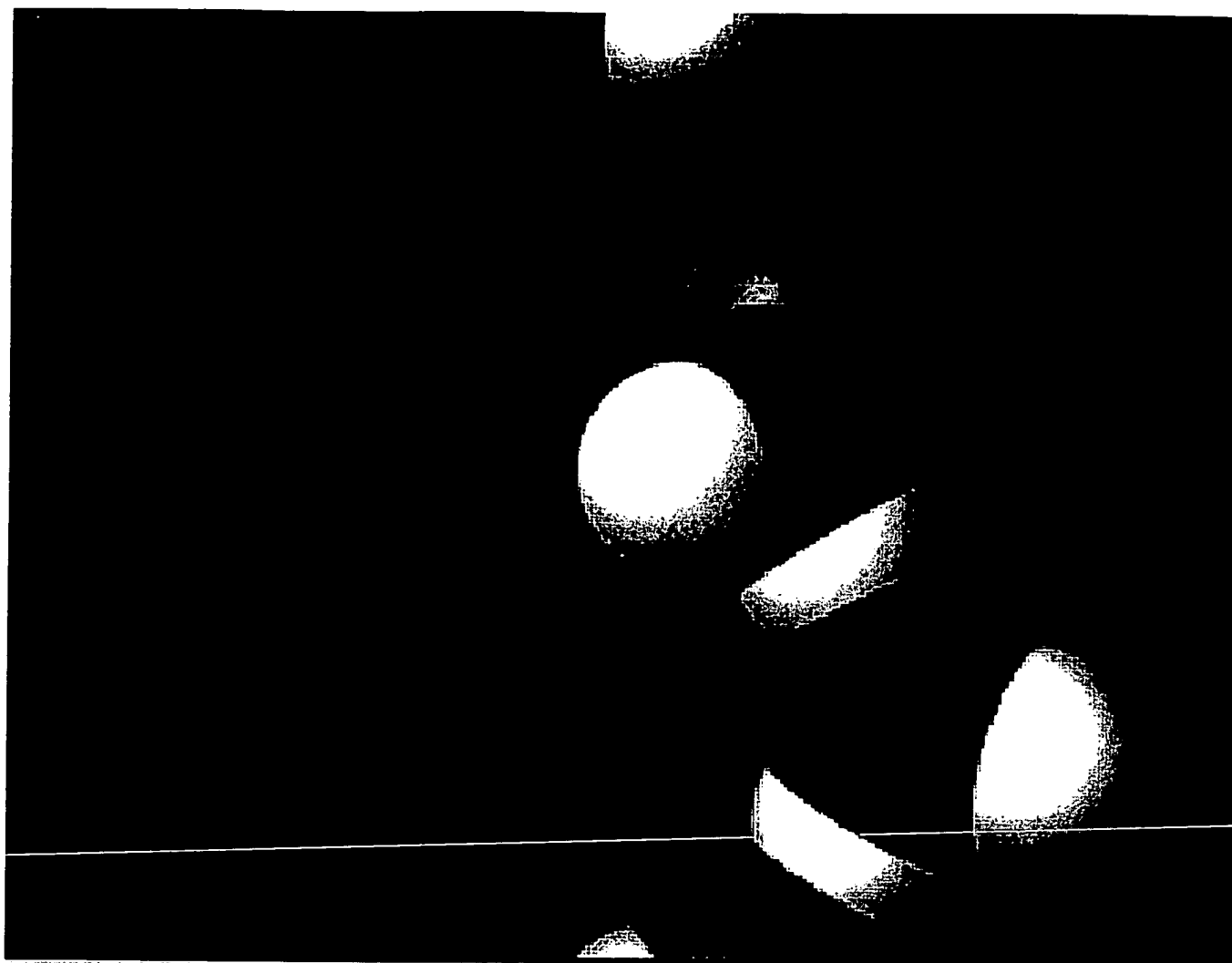ADD COLOR, LAYER BY LAYER — 430

RENDER — 432

FINAL IMAGE — 434

Fig. 4B

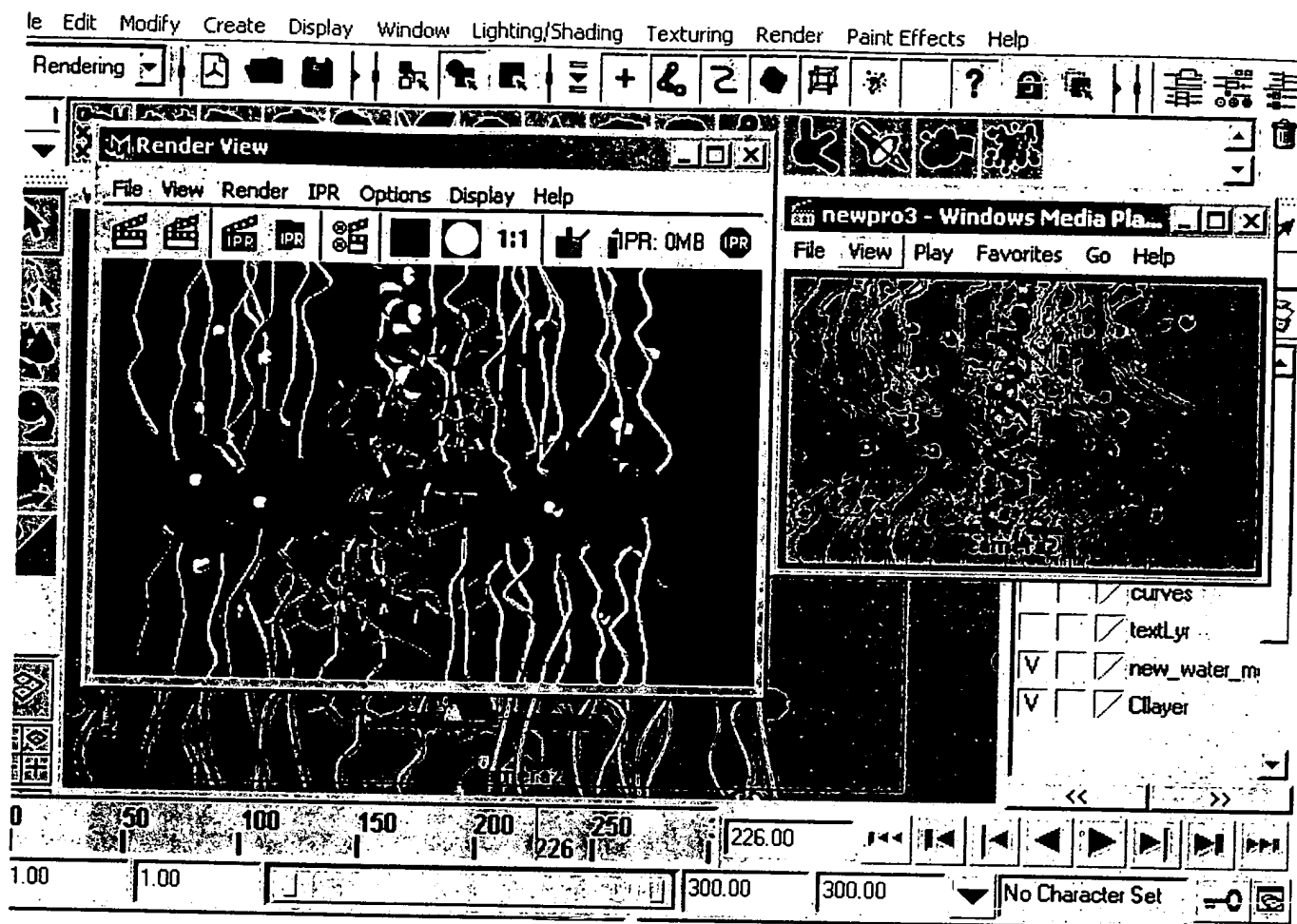The Perspective View of the Water Molecules in the Rendering Sequence

FIG. 6

FIG. 5